18

ELECTRON CAPTURE BY PROTONS FROM HYDROGEN MOLECULES

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The coupled differential equations for calculating the cross section for the process $p+H_2 \rightarrow H+H_2^+$ obtained by using the impact parameter formulation with a two-state approximation (in atomic units) are

$$F_{11}A+2^{\frac{1}{2}}(F_{11}-\tfrac{1}{2}\,i\dot{f}_{11})B-i\dot{A}-2^{\frac{1}{2}}if_{11}\dot{B}=0 \qquad (1)$$

$$2^{\frac{1}{2}}(F_{11}-\tfrac{1}{2}\,i\dot{f}_{11})A+(F_{11}+F_{12}-\tfrac{1}{2}\,i\dot{f}_{12})B-2^{\frac{1}{2}}if_{11}\dot{A}-i(1+f_{12})\dot{B}=0. \quad .. \quad (2)$$

The derivation of the above equations and the expressions for the coefficients F_{ii} etc can be found in our earlier work (Sural and Sil, 1965). With the initial conditions $A(t=-\infty)=1, B(t=-\infty)=0, |B(t=\infty)|^2$ denotes the probability for electron capture by protons from hydrogen molecule. Previously we solved for B using approximations that amount to the neglect of distortion and back-coupling between the final and the initial state. Unitarity was not satisfied and for small impact parameters we had to replace $|B(\infty)|^2$ by half on the average. In view of the importance of the distortion and back-coupling found in other electron capture processes when the incident energy is not too high (cf. Green *et al*, 1965) we have now numerically solved equations. (1) and (2) on an electronic computer. For the low to moderate energies of the incident proton we neglect the effect of momentum transfer. We then write

$$F_{ii}=G_{ii},\ F_{i1}=G_{i1}\exp[i\epsilon t],\ F_{11}=G_{11},\ F_{12}=G_{12}, \qquad .. \quad (3)$$

$$f_{i1}=g_{i1}\exp[i\epsilon t],\ f_{12}=g_{12}.$$

The coefficients G_{ij} etc are all real functions of the distances between the incident proton and the nuclei of the hydrogen molecule and ϵ is the differeni cen energy between the initial and final states. The G_{ii}'s involve some integrals that can be analytically evaluated and others for which Mulliken type approximations have been used. Introducing now the transformations

$$C=A\exp[-i\epsilon t/2] \text{ and } D=B\exp[i\epsilon t/2] \qquad .. \quad (4)$$

and writing $vt = s$ where v is the velocity of the incident proton we obtain the equations

$$Q\frac{dC}{ds} = \left[i\frac{G_1 - G_2G_3}{v} + g_{t_1}\frac{dg_{t_1}}{ds}\right]C + 2^{\frac{1}{2}}\left[i\frac{g_{t_1}G_4 - G_2G_{t_1}}{v} - \frac{1}{2}G_2\frac{dg_{t_1}}{ds} + \frac{1}{2}g_{t_1}\frac{dg_{12}}{ds}\right]D \quad .. \quad (5)$$

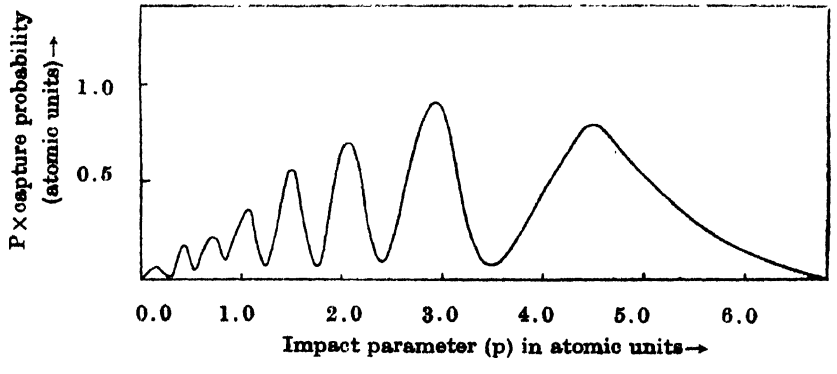
$$Q\frac{dD}{ds} = 2^{\frac{1}{2}}\left[i\frac{g_{t_1}G_3 - G_{t_1}}{v} - \frac{1}{2}\frac{dg_{t_1}}{ds}\right]C + \left[i\frac{G_1 - G_4}{v} + g_{t_1}\frac{dg_{t_1}}{ds} - \frac{1}{2}\frac{dg_{12}}{ds}\right]D \quad .. \quad (6)$$

where

$$Q = 1+g_{12}-2g_{t_1}^2.\ G_1 = 2g_{t_1}G_{t_1},\ G_2 = 1+g_{12},\ G_3 = G_{tt} + \epsilon/2,\ G_4 = G_{11}+G_{12}-G_2\epsilon/2.$$

Starting with the initial conditions $C(s) = 1$, $D(s) = 0$ for a large negative value of s the equations (5) and (6) are then solved for different sets of values of v and p (impact parameter) using the fourth order Runge-Kutta method with automatic step-size adjustment so that unitarity is always satisfied to a specified accuracy. $|D(s)|^2$ for a large positive value of s gives the required capture probability $|B(\infty)|^2$.

The coefficients G_{tt} etc depend upon the orientation of the internuclear axis of the hydrogen molecule. To take account of this effect we have calculated, for each set of values of v and p, the capture probability for the following three different orientations of this axis : (a) parallel to $\vec{v}$ (b) perpendicular to $\vec{v}$ but in the plane of $\vec{v}$ and G (centre of mass of the molecule) and (c) perpendicular to the plane of $\vec{v}$ and G. Taking average for these three orientations the probability for electron capture obtained for protons of energy 1 keV is shown in figure 1 as a function of the impact parameter.



The total cross section for electron capture by protons from hydrogen molecule can be found out from the formula

$$Q = 2\pi \int_0^\infty |B(\infty)|^2 p dp.$$

The value of this cross section at an incident energy of 1 keV is 3.93×10^{-16} cm^2. This compares well with the recent experimental value $\sim 4.3 \times 10^{-16}$ cm^2 obtained by Koopman (1967).

Details of our calculations and results will be published elsewhere.

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19

INFRARED ABSORPTION SPECTRA OF GUAIACOL

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Though the possibility of intramolecular hydrogen bond in guaiacol molecule was not discussed by early authors (Wulf and Liddel, 1935; Pauling, 1936), Batuev (1945), Baker and Shulgin (1958) and Korobkov (1960) later commented on the possibility of existence of a weak intramolecular bond in the molecule. Richards and Walker (1961), however, observed that this bond may not be very weak.

None of these authors apparently compared the absorption spectrum of the pure liquid with the spectra of solutions. In some previous investigations on *o*-chlorophenol (Sirkar *et al*, 1958) and *o*-bromophenol (Banerjee and Chakraborty, 1961) it was observed that in the liquid state mostly dimers formed through intermolecular bond are present. Further, it was observed in the case of hydroxy phenols (Mukherjee and Banerjee, 1967) that in strong proton accepting solvent intermolecular bond between phenols and solvent molecules takes place. In view of these facts, it was thought worthwhile to study the influence of different solvents and mixed solvent on the OH vibrational band of guaiacol and the results of such an investigation have been reported in the present note.